How Can Air Quality Models Provide Detailed Source Attribution and Component Distributions?

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research and development

Science Question

Traditional methods for directly calculating source contributions to airborne particulate matter (PM) concentrations work for primary PM at locations where measurements are available.

In reality, most people do not have monitors located in their homes or offices, and over half the airborne PM in a typical polluted area is secondary (produced by chemical reactions in the atmosphere).

Can a new approach be developed that reveals source contributions to PM and size-resolved chemical composition of PM for use in exposure assessment and health research?

Research Goals

The general goal of this research is to develop an advanced source-oriented air quality model framework that can be used for the source apportionment of primary and secondary PM.

Specific research goals include:

- Develop a general methodology for source apportionment of primary and secondary particulate matter within a source-oriented air quality model.
- Apply the new source apportionment model to regions in California (SoCal and SJV) and the Midwestern US (St. Louis) to identify major sources and size-resolved chemical composition.
- Perform population-weighted exposure assessment and potentially combine with morbidity and mortality data in epidemiological studies.
- In the future, use results of source apportionment and size-resolved chemical composition to guide and interpret source-based health outcome results.

Methods/Approach

The source-oriented air quality model tracks primary particles emitted form different sources separately through the atmosphere. Gas-phase emissions from different sources are also tracked separately so that contributions to secondary PM can be calculated. A fully coupled gas- and particle-phase reaction system predicts how primary emissions are transformed in the atmosphere.

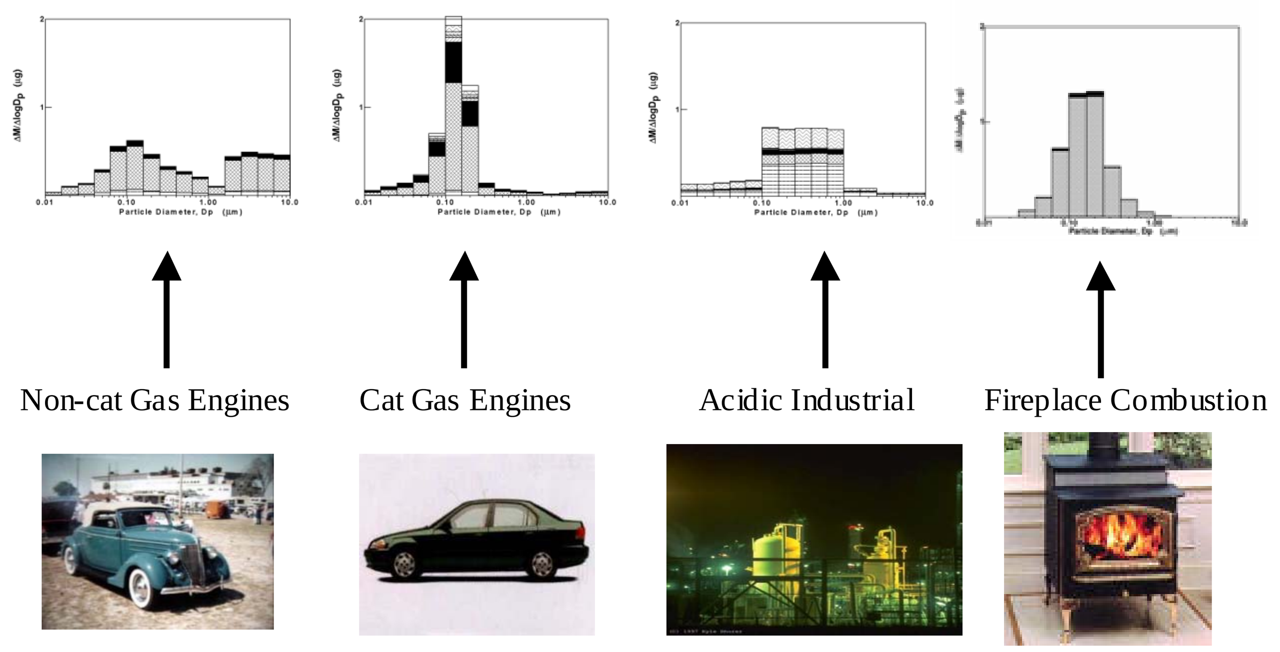


Figure 1: Each emissions source is matched to a size- and composition-resolved profile to provide detailed inputs for the air quality model calculation. Composition profiles for 4 sources are Illustrated above. Other sources not shown include diesel engines, food cooking, paved road dust, crustal sources, sea salt, and study-specific "background particles".

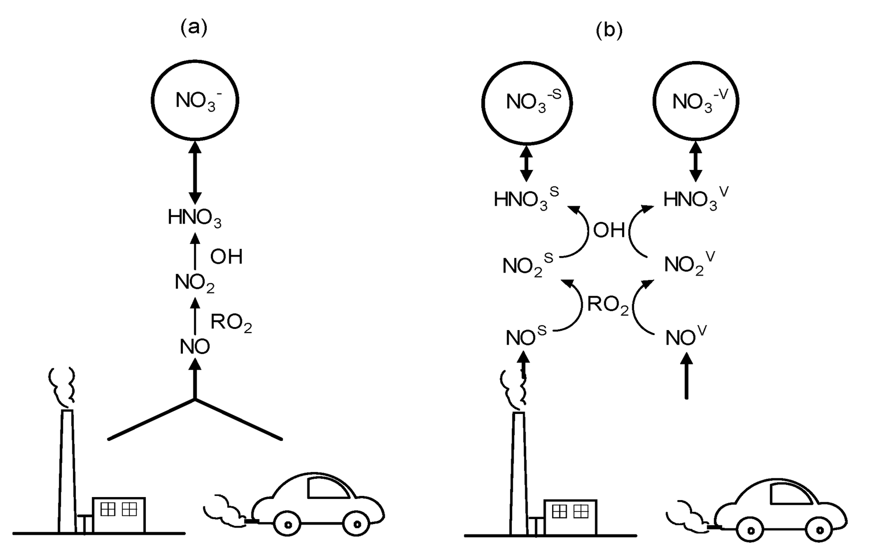
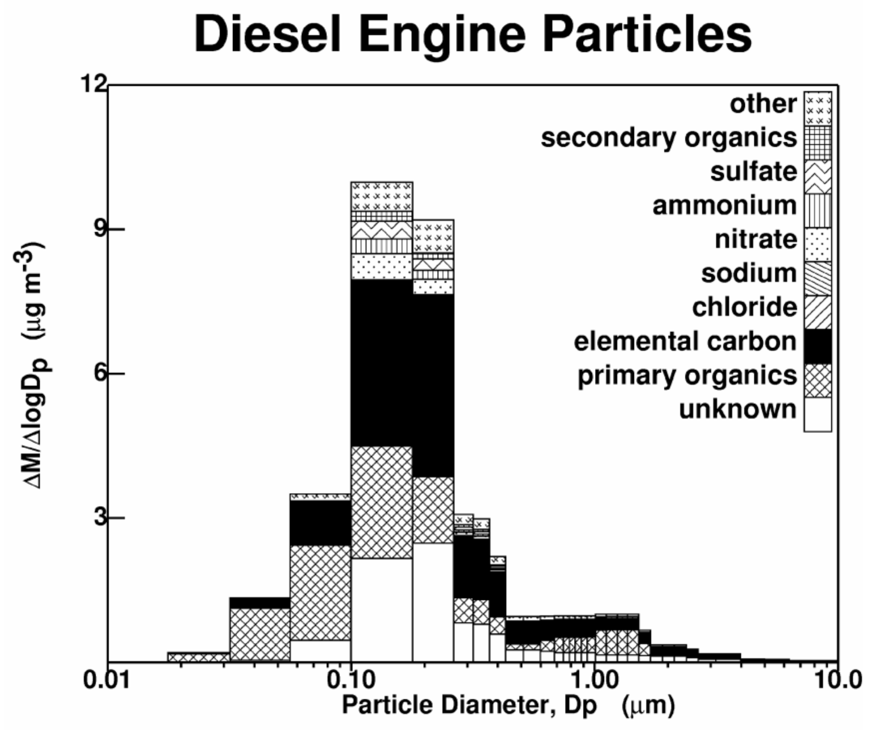


Figure 2: (a)Traditional air quality models combine NO_x emissions from different sources. (b) The source-oriented model retains the source identity of the NO_x in the air quality calculation. By following the NO_x through the gas-phase mechanism, source contributions to secondary nitrate can be calculated. Similar approaches can be used for SO_x, NH_3, and VOC to predict source contributions to sulfate, ammonium ion, and SOA.

The gas-phase chemical reaction mechanism includes basic ozone chemistry, production of condensable inorganic species, as well as detailed reactions describing the oxidation of parent organic compounds leading to the formation of secondary organic aerosol (SOA). The model calculates the dynamic partitioning of 38 SOA species between the gas phase and an aerosol organic phase + aerosol aqueous phase. Activity coefficients are calculated to account for non-ideal solution behavior.

Figure 3: Predicted size and composition distribution of diesel engine particles at Claremont, California on September 9, 1993 after atmospheric processing. Similar plots can be created for particles released from any of the sources tracked by model calculations.



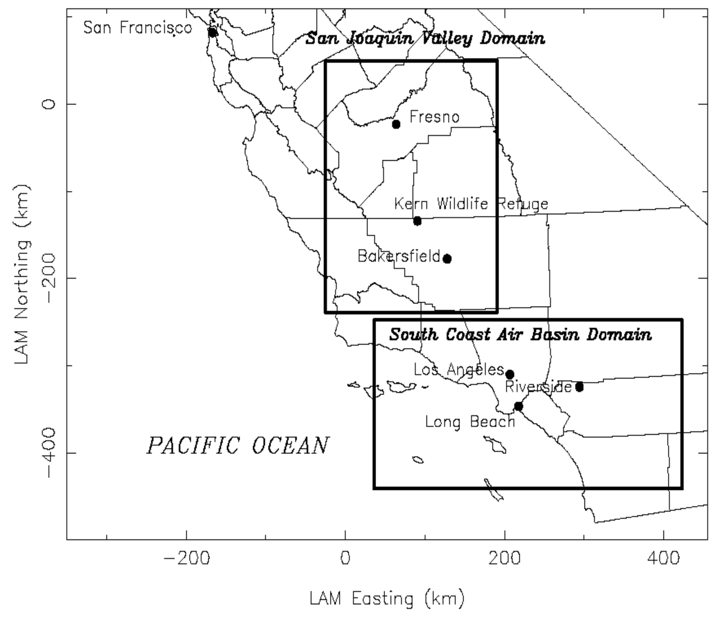


Figure 4: The San Joaquin Valley and South Coast Air Basin domains selected for detailed study.

Results/Conclusions

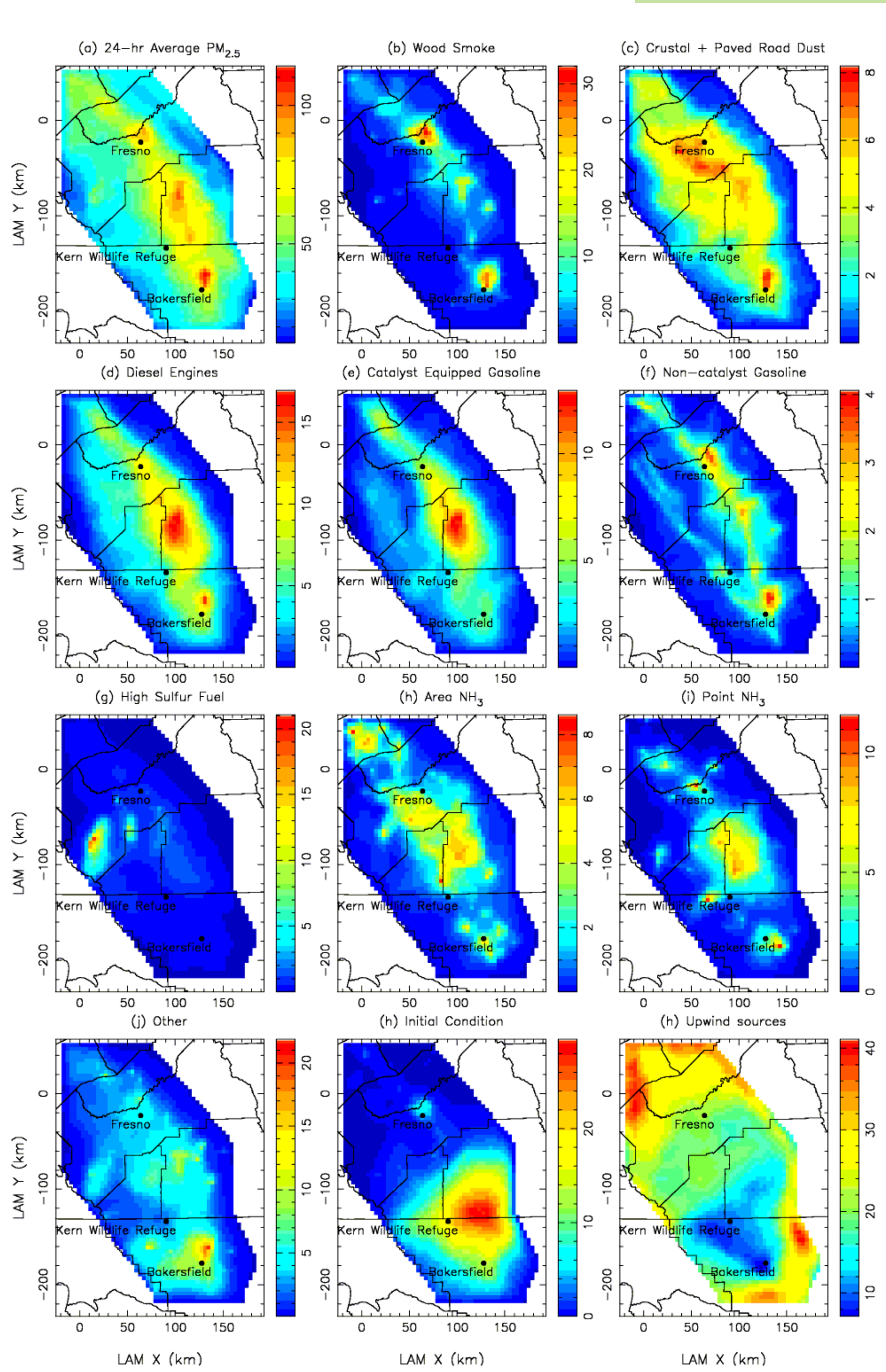


Figure 5: Regional distribution of source contributions to total (primary + secondary) PM2.5 concentrations in the San Joaquin Valley on January 6, 1996. Units are μg m-3.

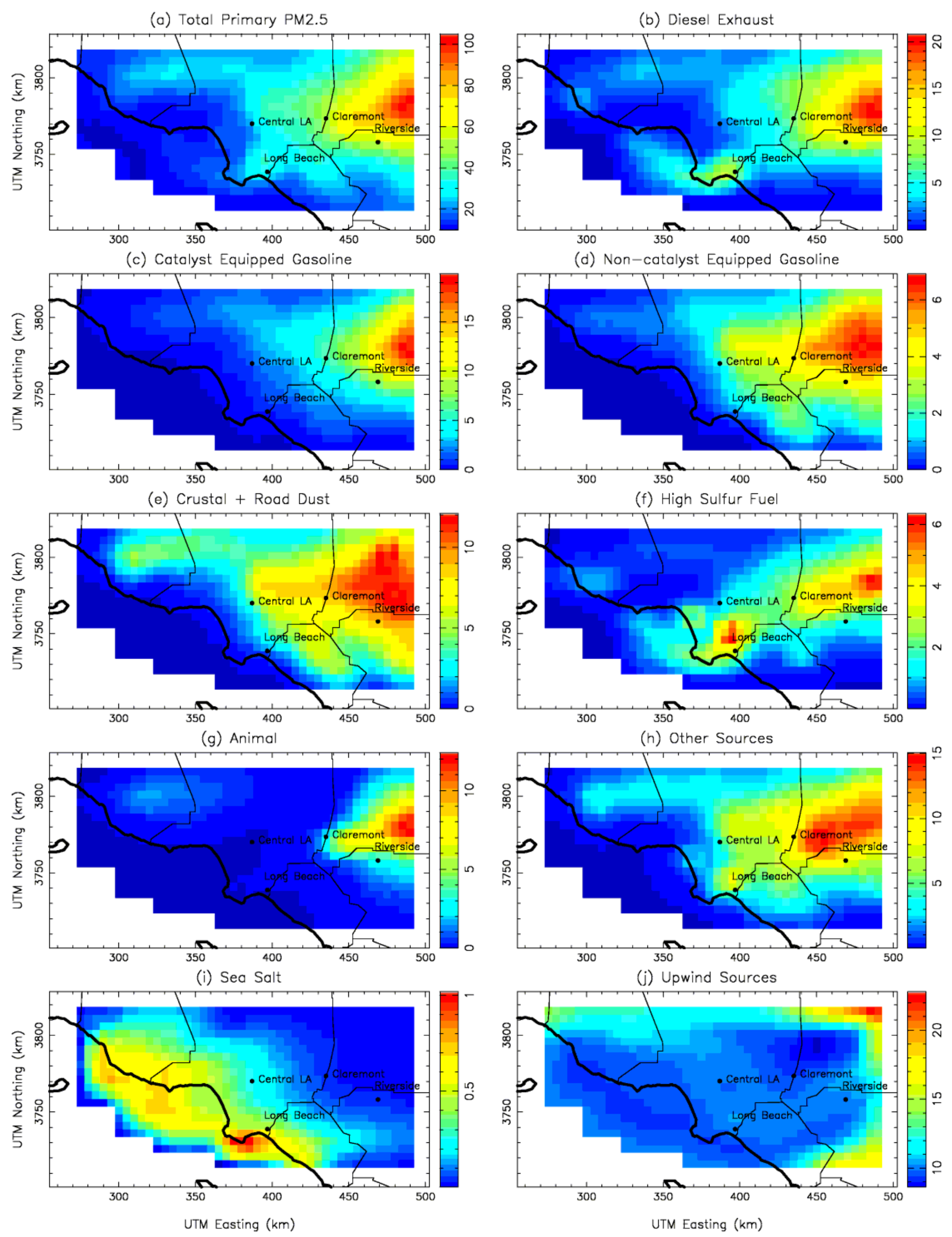


Figure 6: Regional distribution of source contributions to total (primary + secondary) PM2.5 concentrations in the South Coast Air Basin on September 25, 1996. Units are μg m-3.

San Joaquin Valley: The dominant source of $PM_{2.5}$ in the San Joaquin Valley (SJV) was found to be wood smoke "islands" that form around the urban centers. Transportation sources (diesel engines, catalyst-equipped and non-catalyst equipped gasoline engines) contribute significantly to regional ammonium nitrate concentrations with help from area-source (agricultural) ammonia emissions. Approximately 50% of the $PM_{2.5}$ is transported into the SJV from upwind sources that will be resolved in future studies.

South Coast Air Basin: The dominant source of $PM_{2.5}$ in the South Coast Air Basin was found to be transportation sources (diesel engines, catalyst and non-catalyst equipped gasoline engines). A plume of acidic sulfate particles is formed downwind of the industrial area adjacent to Long Beach.

Future Directions

The regional source contribution plots shown to the left can be created for any combination of size fraction and chemical component of PM. The model can be run for historical time periods and the results can be combined with census data to calculate population-weighted exposures to particles emitted from different sources. Historical morbidity and mortality data can then be correlated to the results to identify sources of particulate matter with adverse health effects.

Impact and Outcomes

The largest sources of total PM2.5 (primary + secondary) have been identified for the two most heavily polluted areas in the United States: the South Coast Air Basin and the San Joaquin Valley.

The different spatial distributions demonstrate the difficulty of using only a small number of speciation measurement sites to characterize exposure.

This research builds to population-weighted exposure studies that can help identify sources and compositions of airborne particles that harm human health.

The modeling tool enables tracking the spatial and temporal distributions of source attributed components of PM at 5 km resolution.

Source to Outcome